Substituent Effect on Triplet State Aromaticity of Benzene

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Supporting Information

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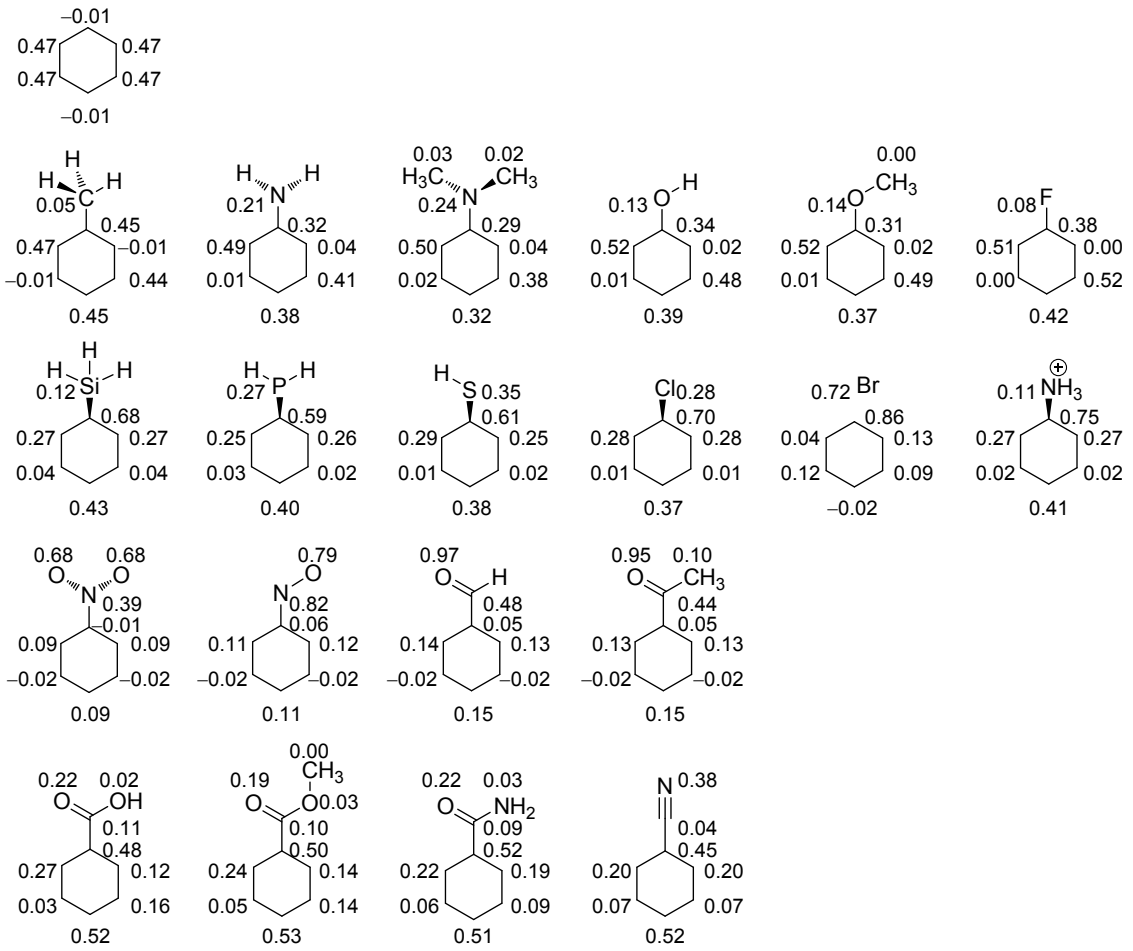

Figure S1. Spin densities at heavy atoms obtained by the Hirshfeld population analysis.

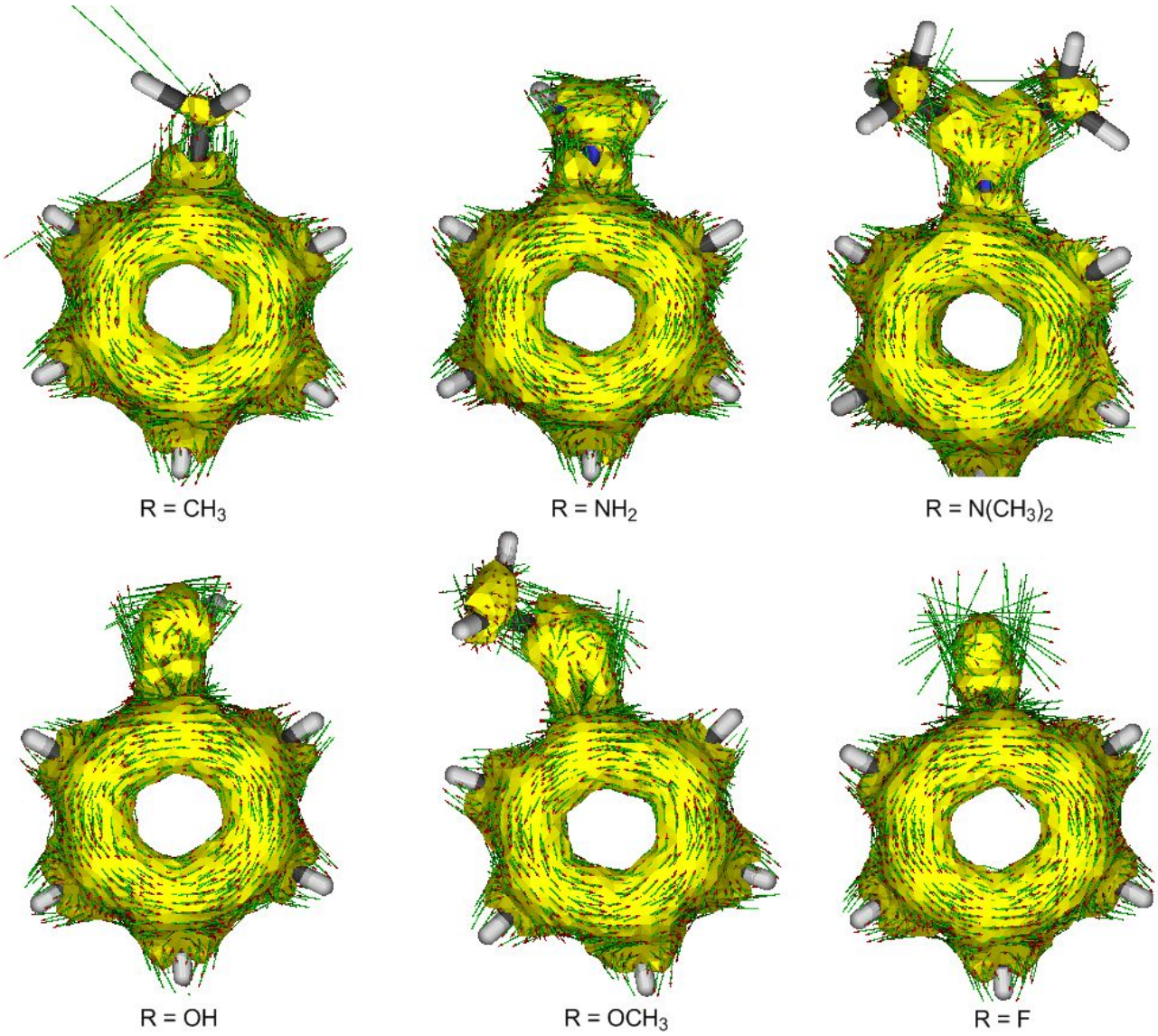

Figure S2. ACID plots of benzenes substituted with σ- and π-electron donating groups. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

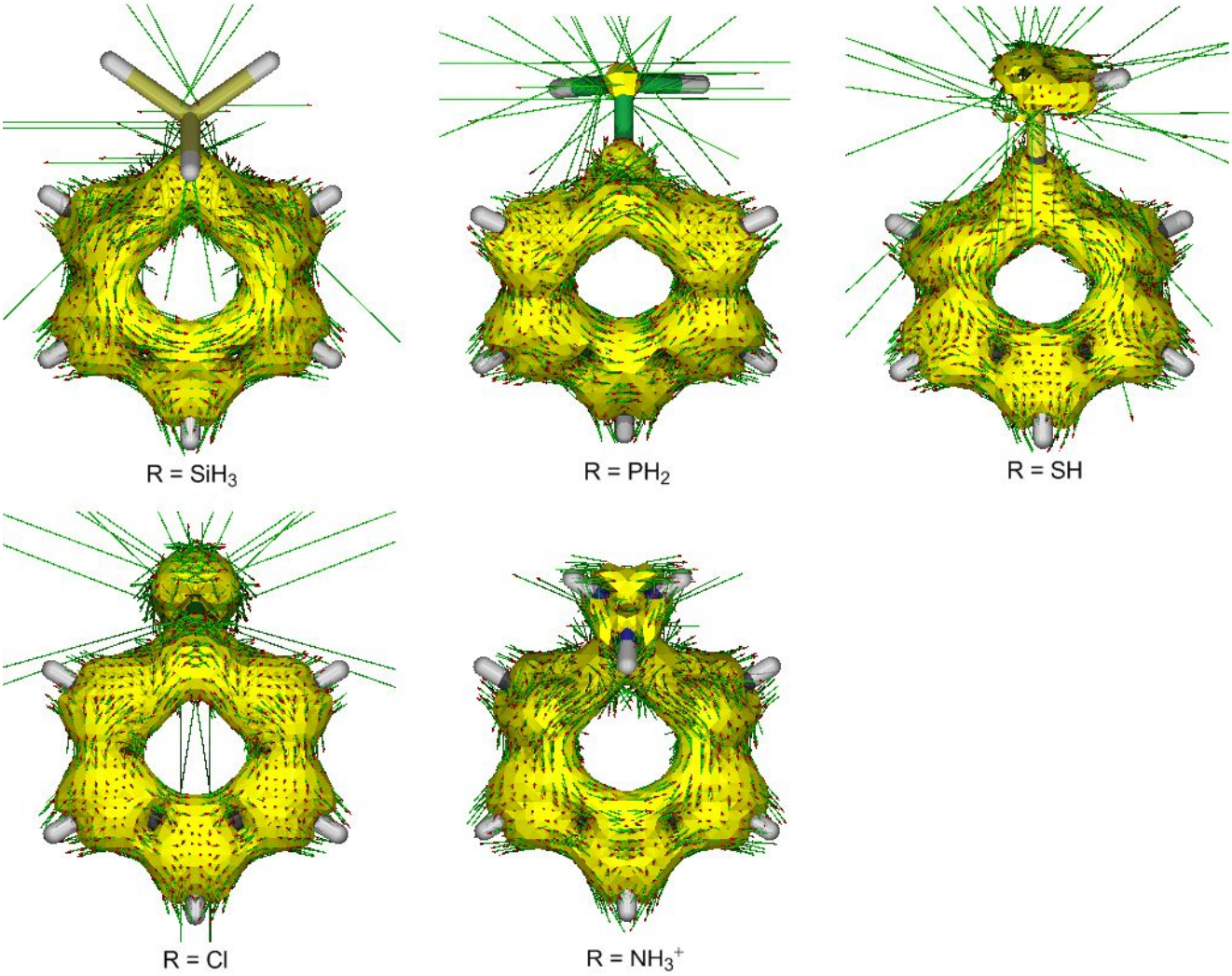

Figure S3. ACID plots of benzenes substituted with groups containing the third row elements and σ-electron accepting NH_3^+ group. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

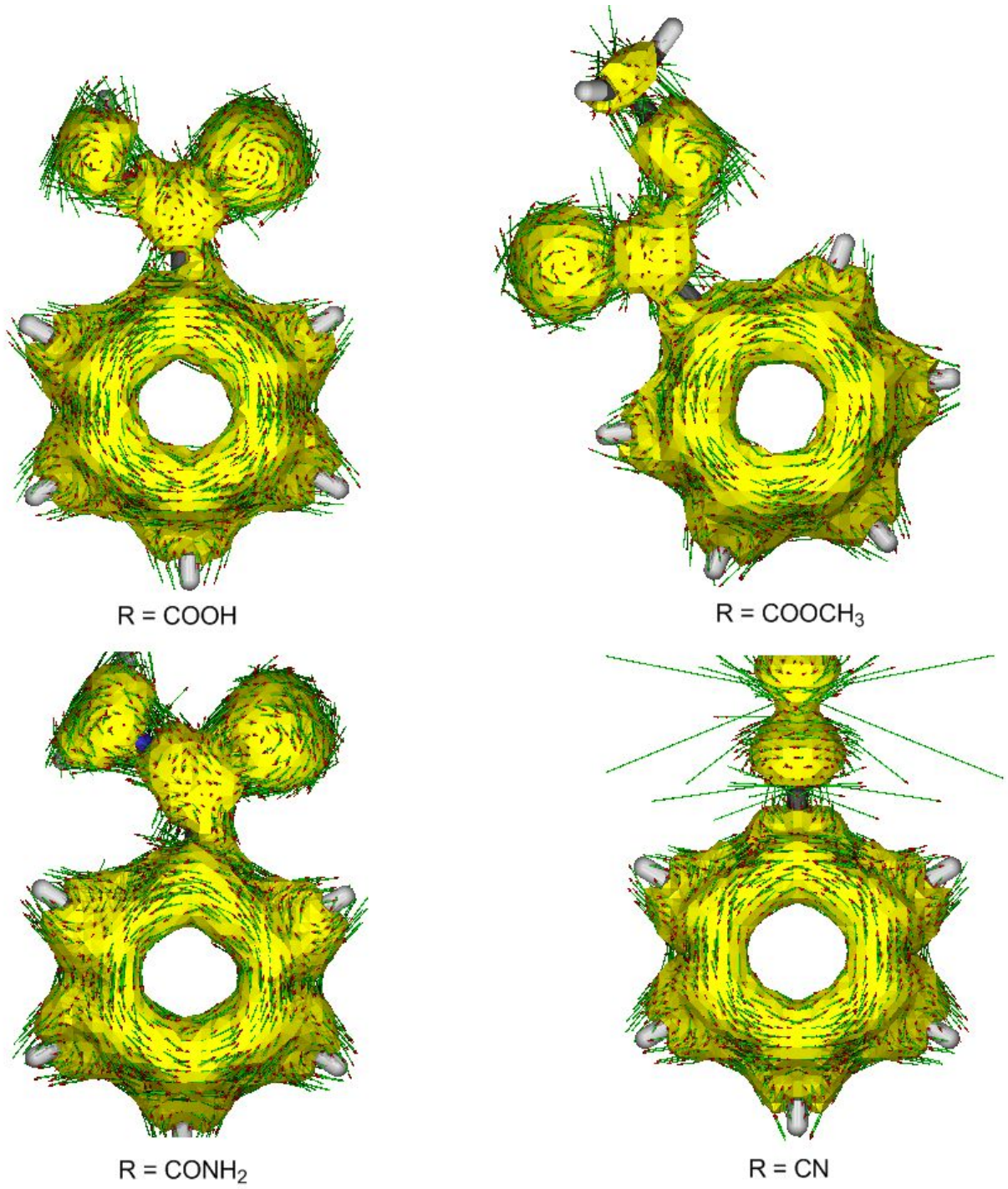

Figure S4. ACID plots of benzenes substituted with π-electron accepting groups. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

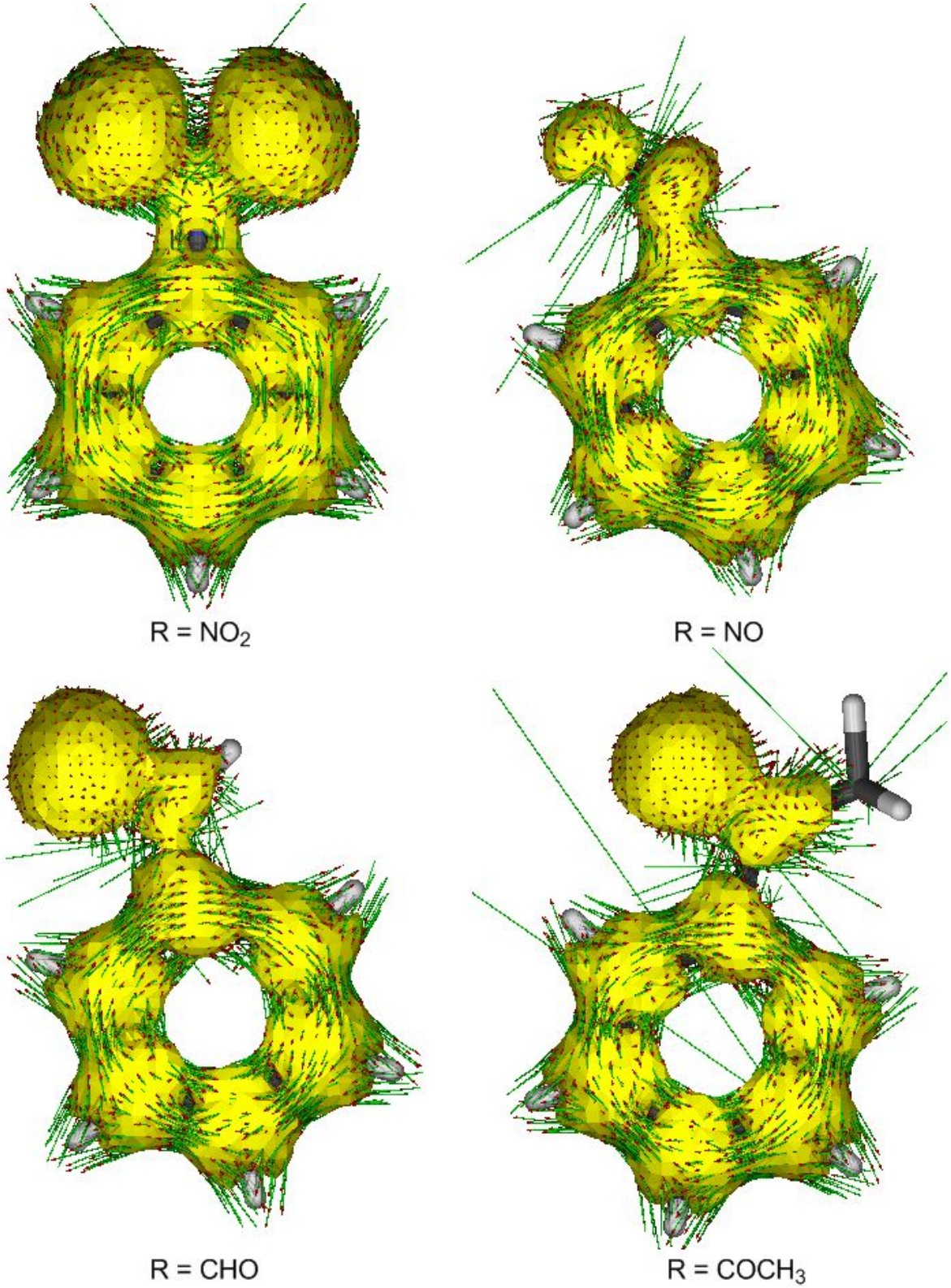

Figure S5. ACID plots of benzenes substituted with π-electron accepting groups. Clockwise circulation is diatropic and counterclockwise circulation is paratropic.

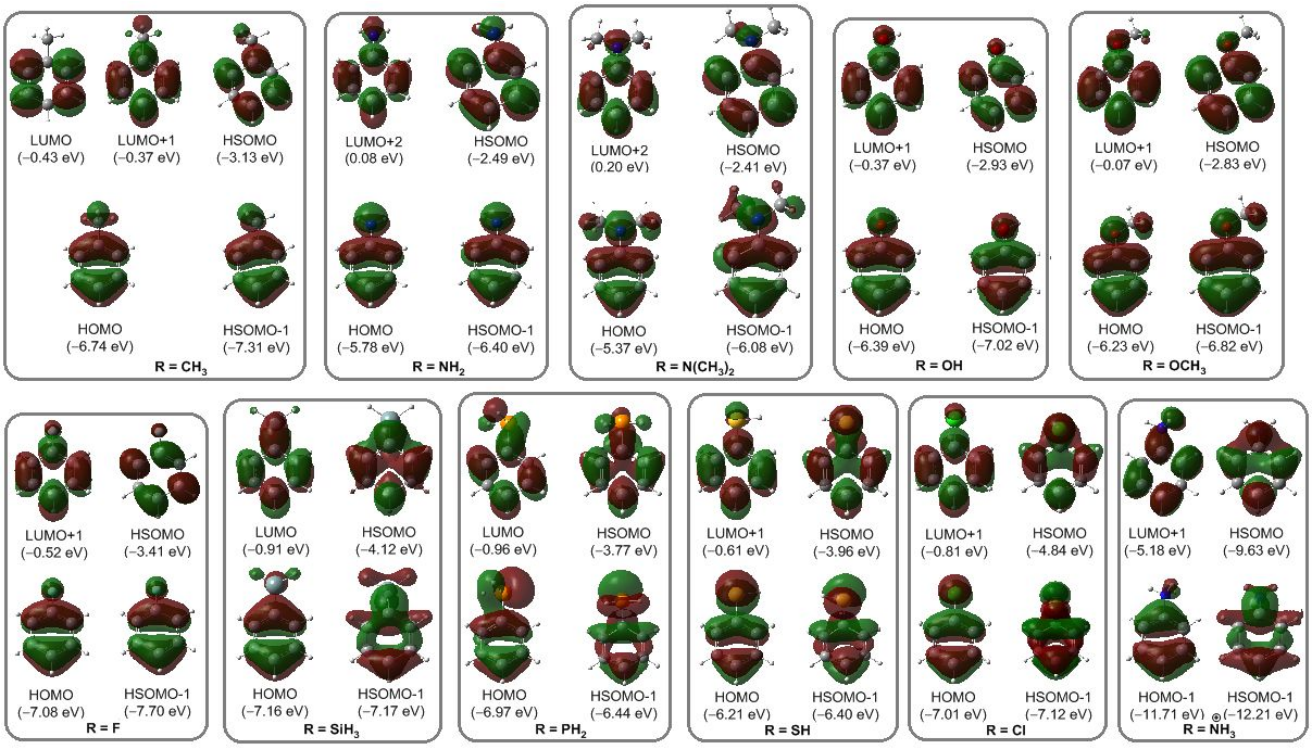

Figure S6. Molecular orbitals involved in the most important $S_0 \rightarrow T_1$ excitation of compounds containing σ- or π-electron donating substituents and electron-accepting NH_3^+ group, at an isovalue of 0.03 a.u.

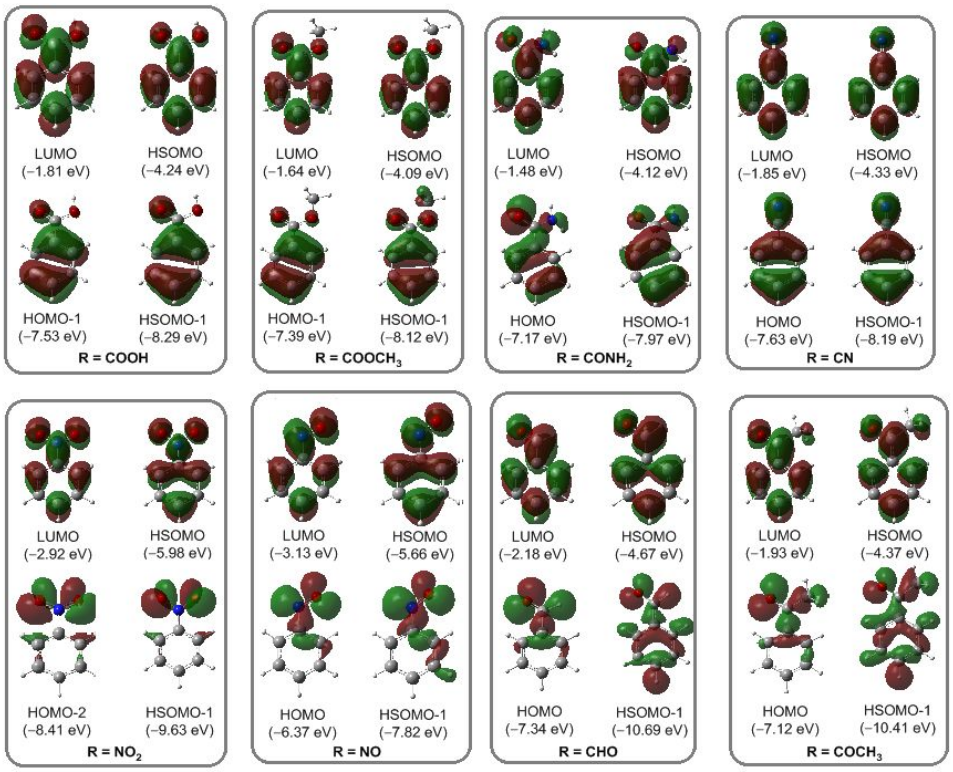

Figure S7. Molecular orbitals involved in the most important $S_0 \rightarrow T_1$ excitation of compounds containing π-electron accepting substituents, at an isovalue of 0.03 a.u.

Absolute energies (a.u.) and x, y, z coordinates of optimized structures

Benzene S_0

E = -232.3112416 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.394301	0.000000
2	6	0	1.207500	0.697151	0.000000
3	6	0	1.207500	-0.697151	0.000000
4	6	0	0.000000	-1.394301	0.000000
5	6	0	-1.207500	-0.697151	0.000000
6	6	0	-1.207500	0.697151	0.000000
7	1	0	0.000000	2.478574	0.000000
8	1	0	2.146508	1.239287	0.000000
9	1	0	2.146508	-1.239287	0.000000
10	1	0	0.000000	-2.478574	0.000000
11	1	0	-2.146508	-1.239287	0.000000
12	1	0	-2.146508	1.239287	0.000000

Benzene T_1

E = -232.1699199 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.207797	0.759712
2	6	0	0.000000	0.000000	1.441395
3	6	0	0.000000	-1.207797	0.759712
4	6	0	0.000000	-1.207797	-0.759712
5	6	0	0.000000	0.000000	-1.441395
6	6	0	0.000000	1.207797	-0.759712
7	1	0	0.000000	2.152534	1.287125
8	1	0	0.000000	0.000000	2.526694
9	1	0	0.000000	-2.152534	1.287125
10	1	0	0.000000	-2.152534	-1.287125
11	1	0	0.000000	0.000000	-2.526694
12	1	0	0.000000	2.152534	-1.287125

R = CH_3 S_0

E = -271.6388137 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.007555	-1.199548	1.203415
2	6	0	-0.007555	0.194230	1.200484
3	6	0	-0.004273	0.913135	0.000000
4	6	0	-0.007555	0.194230	-1.200484
5	6	0	-0.007555	-1.199548	-1.203415
6	6	0	-0.006636	-1.902681	0.000000
7	1	0	-0.012150	-1.736113	2.146085
8	1	0	-0.012602	0.732057	2.143638
9	1	0	-0.012602	0.732057	-2.143638
10	1	0	-0.012150	-1.736113	-2.146085
11	1	0	-0.009469	-2.986956	0.000000
12	6	0	0.029022	2.423022	0.000000
13	1	0	1.060711	2.792130	0.000000
14	1	0	-0.464553	2.832953	-0.884499
15	1	0	-0.464553	2.832953	0.884499

R = CH_3 T_1

E = -271.5030272 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.339444	-1.082552	0.000000
2	6	0	-1.235172	0.296005	0.000000
3	6	0	0.000000	0.941723	0.000000
4	6	0	1.260974	0.082772	0.000000
5	6	0	1.155015	-1.302155	0.000000
6	6	0	-0.082614	-1.922438	0.000000
7	1	0	-2.303040	-1.574292	0.000000
8	1	0	-2.139355	0.898483	0.000000
9	1	0	2.224891	0.576320	0.000000
10	1	0	2.056460	-1.906817	0.000000
11	1	0	-0.168229	-3.001476	0.000000
12	6	0	0.174674	2.415347	0.000000
13	1	0	0.754391	2.745357	0.876697
14	1	0	0.754391	2.745357	-0.876697
15	1	0	-0.780104	2.944855	0.000000

R = NH_2 S_0

E = -287.6876274 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.003385	-1.170662	1.200866
2	6	0	-0.003385	0.220540	1.206220
3	6	0	-0.002114	0.937027	0.000000
4	6	0	-0.003385	0.220540	-1.206220
5	6	0	-0.003385	-1.170662	-1.200866
6	6	0	-0.003246	-1.879746	0.000000
7	1	0	-0.002925	-1.703712	2.145552
8	1	0	-0.008922	0.759878	2.148457
9	1	0	-0.008922	0.759878	-2.148457
10	1	0	-0.002925	-1.703712	-2.145552
11	1	0	-0.002727	-2.963107	0.000000
12	7	0	-0.059499	2.334027	0.000000
13	1	0	0.278153	2.785185	0.837363
14	1	0	0.278153	2.785185	-0.837363

R = NH_2 T_1

E = -287.5601692 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.140663	1.279372	0.000995
2	6	0	0.252651	1.251762	-0.008653
3	6	0	0.942462	0.047299	-0.005892
4	6	0	0.201310	-1.264412	-0.001768
5	6	0	-1.202797	-1.219895	0.007646
6	6	0	-1.873644	-0.018885	0.009858
7	1	0	-1.689122	2.209789	0.014599
8	1	0	0.815723	2.181328	-0.002241
9	1	0	0.752974	-2.188776	-0.113364
10	1	0	-1.764047	-2.148262	-0.001800
11	1	0	-2.957558	-0.006533	0.009642
12	7	0	2.309867	-0.053131	-0.043108
13	1	0	2.863210	0.780943	0.091202
14	1	0	2.733829	-0.908013	0.290602

R = $N(CH_3)_2$ S_0

E = -366.3140525 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037327	-1.942171	1.196632
2	6	0	-0.025281	-0.552644	1.206038
3	6	0	-0.072515	0.180711	0.000000
4	6	0	-0.025281	-0.552644	-1.206038
5	6	0	0.037327	-1.942171	-1.196632
6	6	0	0.066109	-2.655162	0.000000
7	1	0	0.068794	-2.470620	2.143622
8	1	0	-0.038481	-0.041089	2.158308
9	1	0	-0.038481	-0.041089	-2.158308
10	1	0	0.068794	-2.470620	-2.143622
11	1	0	0.117267	-3.737278	0.000000
12	7	0	-0.176471	1.569024	0.000000
13	6	0	0.037327	2.295981	-1.240748
14	1	0	-0.680325	1.985951	-2.004873
15	1	0	-0.119060	3.359090	-1.060040
16	1	0	1.051061	2.160079	-1.647521
17	6	0	0.037327	2.295981	1.240748
18	1	0	-0.119060	3.359090	1.060040
19	1	0	-0.680325	1.985951	2.004873
20	1	0	1.051061	2.160079	1.647521

R = $N(CH_3)_2$ T_1

E = -366.191025 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.895952	1.273138	-0.186217
2	6	0	0.505168	1.229099	-0.127142
3	6	0	-0.181445	0.025341	0.037688
4	6	0	0.596960	-1.255446	0.205738
5	6	0	2.009430	-1.180761	0.146443
6	6	0	2.654966	0.009794	-0.053276
7	1	0	2.417073	2.201194	-0.373807
8	1	0	-0.053337	2.146840	-0.270928
9	1	0	0.118137	-2.109435	0.668732
10	1	0	2.586975	-2.087538	0.295104
11	1	0	3.738010	0.039453	-0.096532
12	7	0	-1.553140	-0.060780	0.153272
13	6	0	-2.274986	-1.193956	-0.418383
14	1	0	-1.638855	-2.075904	-0.439290
15	1	0	-3.170745	-1.398790	0.172211
16	1	0	-2.578990	-0.977995	-1.453300
17	6	0	-2.348983	1.145999	0.296562
18	1	0	-3.344575	0.872363	0.650444
19	1	0	-1.885168	1.812916	1.023083
20	1	0	-2.458932	1.683113	-0.657102

R = OH S_0

E = -307.5586319 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.187840	-1.162180	0.000000
2	6	0	-1.204282	0.231745	0.000000
3	6	0	0.000000	0.938152	0.000000
4	6	0	1.215579	0.252752	0.000000
5	6	0	1.218472	-1.138781	0.000000
6	6	0	0.020797	-1.855110	0.000000
7	1	0	-2.126623	-1.704651	0.000000
8	1	0	-2.148862	0.767950	0.000000
9	1	0	2.138691	0.819413	0.000000
10	1	0	2.165531	-1.666804	0.000000
11	1	0	0.030124	-2.938376	0.000000
12	8	0	0.050909	2.307122	0.000000
13	1	0	-0.842490	2.666024	0.000000

R = OH T_1

E = -307.4245929 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.319910	-1.062978	0.000000
2	6	0	-1.229903	0.337547	0.000000
3	6	0	0.000000	0.950038	0.000000
4	6	0	1.280097	0.158783	0.000000
5	6	0	1.178709	-1.244107	0.000000
6	6	0	-0.044998	-1.864449	0.000000
7	1	0	-2.274592	-1.567997	0.000000
8	1	0	-2.133382	0.942190	0.000000
9	1	0	2.219234	0.692434	0.000000
10	1	0	2.084988	-1.840088	0.000000
11	1	0	-0.112010	-2.945638	0.000000
12	8	0	0.208644	2.289360	0.000000
13	1	0	-0.637360	2.755207	0.000000

R = OCH_3 S_0

E = -346.867558 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.468256	1.840225	0.000000
2	6	0	0.925274	0.519602	0.000000
3	6	0	0.000000	-0.527780	0.000000
4	6	0	-1.371877	-0.245894	0.000000
5	6	0	-1.809657	1.071373	0.000000
6	6	0	-0.892394	2.125887	0.000000
7	1	0	1.192245	2.647592	0.000000
8	1	0	1.989156	0.324851	0.000000
9	1	0	-2.071031	-1.073386	0.000000
10	1	0	-2.874213	1.277553	0.000000
11	1	0	-1.237014	3.153026	0.000000
12	8	0	0.332799	-1.852429	0.000000
13	6	0	1.708306	-2.207905	0.000000
14	1	0	2.218390	-1.833356	0.894440
15	1	0	1.734237	-3.296548	0.000000
16	1	0	2.218390	-1.833356	-0.894440

R = OCH_3 T_1

E = -346.7360259 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756297	1.770839	0.000000
2	6	0	1.034253	0.390829	0.000000
3	6	0	0.000000	-0.515527	0.000000
4	6	0	-1.436697	-0.067225	0.000000
5	6	0	-1.699590	1.318121	0.000000
6	6	0	-0.675462	2.226133	0.000000
7	1	0	1.552057	2.501549	0.000000
8	1	0	2.064046	0.055990	0.000000
9	1	0	-2.208902	-0.822688	0.000000
10	1	0	-2.728346	1.662101	0.000000
11	1	0	-0.882749	3.289535	0.000000
12	8	0	0.099570	-1.860396	0.000000
13	6	0	1.397624	-2.450373	0.000000
14	1	0	1.955758	-2.156806	0.894256
15	1	0	1.237271	-3.526487	0.000000
16	1	0	1.955758	-2.156806	-0.894256

R = **F** S_0

E = -331.5801119 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.206735	-1.134261
2	6	0	0.000000	1.215919	0.259986
3	6	0	0.000000	0.000000	0.925927
4	6	0	0.000000	-1.215919	0.259986
5	6	0	0.000000	-1.206735	-1.134261
6	6	0	0.000000	0.000000	-1.833179
7	1	0	0.000000	2.147659	-1.672595
8	1	0	0.000000	2.138900	0.826391
9	1	0	0.000000	-2.138900	0.826391
10	1	0	0.000000	-2.147659	-1.672595
11	1	0	0.000000	0.000000	-2.916679
12	9	0	0.000000	0.000000	2.282654

R = **F** T_1

E = -331.4402339 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.167409	1.242116	0.000000
2	6	0	-1.281249	-0.155858	0.000000
3	6	0	0.000000	-0.944263	0.000000
4	6	0	1.236890	-0.371206	0.000000
5	6	0	1.336725	1.029609	0.000000
6	6	0	0.063615	1.852759	0.000000
7	1	0	-2.067980	1.846467	0.000000
8	1	0	-2.223973	-0.683166	0.000000
9	1	0	2.118917	-1.000854	0.000000
10	1	0	2.296211	1.525786	0.000000
11	1	0	0.144921	2.932316	0.000000
12	9	0	-0.155504	-2.282165	0.000000

R = SiH_3 S_0

E = -523.0297441 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.012083	-1.650886	-1.205586
2	6	0	0.012083	-0.257050	-1.203262
3	6	0	0.008307	0.466400	0.000000
4	6	0	0.012083	-0.257050	1.203262
5	6	0	0.012083	-1.650886	1.205586
6	6	0	0.011423	-2.350355	0.000000
7	1	0	0.016517	-2.190148	-2.146650
8	1	0	0.019555	0.269697	-2.152758
9	1	0	0.019555	0.269697	2.152758
10	1	0	0.016517	-2.190148	2.146650
11	1	0	0.014255	-3.434847	0.000000
12	14	0	-0.027421	2.348627	0.000000
13	1	0	0.656185	2.864914	-1.214497
14	1	0	-1.423243	2.864114	0.000000
15	1	0	0.656185	2.864914	1.214497

R = SiH_3 T_1

E = -522.8977178 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.641177	1.356728	1.242464
2	6	0	0.641177	-0.002324	1.253854
3	6	0	0.239160	-0.690076	0.000000
4	6	0	0.641177	-0.002324	-1.253854
5	6	0	0.641177	1.356728	-1.242464
6	6	0	0.508913	2.068163	0.000000
7	1	0	0.824761	1.916634	2.154468
8	1	0	0.854948	-0.567952	2.154654
9	1	0	0.854948	-0.567952	-2.154654
10	1	0	0.824761	1.916634	-2.154468
11	1	0	0.512243	3.151082	0.000000
12	14	0	-1.323237	-1.733581	0.000000
13	1	0	-2.573496	-0.918981	0.000000
14	1	0	-1.324773	-2.590353	-1.214932
15	1	0	-1.324773	-2.590353	1.214932

R = PH_2 S_0

E = -574.2803668 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.219185	1.203987	-0.004984
2	6	0	-1.611756	1.212325	0.004682
3	6	0	-2.320802	0.010774	0.012423
4	6	0	-1.629886	-1.197963	0.003085
5	6	0	-0.234900	-1.205249	-0.016514
6	6	0	0.487860	-0.006394	-0.013014
7	1	0	0.319516	2.145205	-0.006063
8	1	0	-2.144160	2.157174	0.008271
9	1	0	-3.404951	0.018984	0.021354
10	1	0	-2.173410	-2.136277	0.003321
11	1	0	0.295522	-2.151435	-0.039348
12	15	0	2.340531	-0.112391	-0.033847
13	1	0	2.591448	1.138081	-0.664785
14	1	0	2.580078	0.409256	1.270880

R = PH_2 T_1

E = -574.1538476 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.246180	1.261386	0.458497
2	6	0	1.494242	1.237069	-0.082553
3	6	0	2.111110	-0.003128	-0.449271
4	6	0	1.490616	-1.239721	-0.088330
5	6	0	0.243283	-1.260404	0.458158
6	6	0	-0.529519	0.002418	0.489989
7	1	0	-0.188406	2.183277	0.830624
8	1	0	2.062559	2.157326	-0.175870
9	1	0	3.109821	-0.003820	-0.867366
10	1	0	2.054653	-2.162329	-0.185563
11	1	0	-0.191112	-2.179521	0.836541
12	15	0	-2.193279	0.011227	-0.193997
13	1	0	-2.108946	0.998864	-1.223967
14	1	0	-2.174855	-1.147923	-1.023396

R = SH S_0

E = -630.5252609 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.199717	-1.593436	0.000000
2	6	0	-1.207154	-0.201310	0.000000
3	6	0	0.000000	0.506116	0.000000
4	6	0	1.209263	-0.196227	0.000000
5	6	0	1.205982	-1.589234	0.000000
6	6	0	0.004685	-2.295475	0.000000
7	1	0	-2.142295	-2.129392	0.000000
8	1	0	-2.150003	0.334196	0.000000
9	1	0	2.152638	0.338098	0.000000
10	1	0	2.150554	-2.121873	0.000000
11	1	0	0.007041	-3.379017	0.000000
12	16	0	-0.083832	2.291378	0.000000
13	1	0	1.245028	2.513343	0.000000

R = SH T_1

E = -630.4034447 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.473075	-1.221963	-0.090693
2	6	0	0.233197	-1.266936	0.465895
3	6	0	-0.556470	-0.019965	0.584030
4	6	0	0.199011	1.251629	0.477180
5	6	0	1.436653	1.248693	-0.097505
6	6	0	2.076523	0.026597	-0.446304
7	1	0	2.044001	-2.136922	-0.214797
8	1	0	-0.198058	-2.204477	0.801571
9	1	0	-0.249913	2.170716	0.840450
10	1	0	1.974028	2.183203	-0.227827
11	1	0	3.065320	0.040855	-0.887109
12	16	0	-2.087932	-0.086529	-0.339526
13	1	0	-2.400403	1.222763	-0.235498

R = Cl S_0

E = -691.9342153 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.205496	-1.572630
2	6	0	0.000000	1.213602	-0.178716
3	6	0	0.000000	0.000000	0.502261
4	6	0	0.000000	-1.213602	-0.178716
5	6	0	0.000000	-1.205496	-1.572630
6	6	0	0.000000	0.000000	-2.272306
7	1	0	0.000000	2.147558	-2.109134
8	1	0	0.000000	2.145223	0.372678
9	1	0	0.000000	-2.145223	0.372678
10	1	0	0.000000	-2.147558	-2.109134
11	1	0	0.000000	0.000000	-3.355963
12	17	0	0.000000	0.000000	2.262665

R = Cl T_1

E = -691.8085574 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574362	1.299462	1.236325
2	6	0	-0.574362	-0.065286	1.258301
3	6	0	-0.325286	-0.784073	0.000000
4	6	0	-0.574362	-0.065286	-1.258301
5	6	0	-0.574362	1.299462	-1.236325
6	6	0	-0.524220	2.004259	0.000000
7	1	0	-0.675517	1.858886	2.160716
8	1	0	-0.688300	-0.624616	2.179580
9	1	0	-0.688300	-0.624616	-2.179580
10	1	0	-0.675517	1.858886	-2.160716
11	1	0	-0.543194	3.087179	0.000000
12	17	0	1.303091	-1.628644	0.000000

R = Br S_0

E = -2805.8538831 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.205469	-2.181859
2	6	0	0.000000	1.214092	-0.787413
3	6	0	0.000000	0.000000	-0.107095
4	6	0	0.000000	-1.214092	-0.787413
5	6	0	0.000000	-1.205469	-2.181859
6	6	0	0.000000	0.000000	-2.881343
7	1	0	0.000000	2.147714	-2.718214
8	1	0	0.000000	2.148078	-0.240320
9	1	0	0.000000	-2.148078	-0.240320
10	1	0	0.000000	-2.147714	-2.718214
11	1	0	0.000000	0.000000	-3.965062
12	35	0	0.000000	0.000000	1.812686

R = Br T_1

E = -2805.7380203 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.152354	1.328713	0.422490
2	6	0	-0.554901	0.286843	1.173348
3	6	0	-1.007519	-0.999633	0.915069
4	6	0	-1.960121	-1.345587	-0.008640
5	6	0	-2.529304	-0.293018	-0.739800
6	6	0	-2.123402	1.031840	-0.520961
7	1	0	-0.838507	2.351940	0.593194
8	1	0	0.121947	0.505827	1.989172
9	1	0	-2.261743	-2.372769	-0.176801
10	1	0	-3.286285	-0.509594	-1.486161
11	1	0	-2.575089	1.830142	-1.097726
12	35	0	1.851579	-0.053157	-0.207735

R = NH_3^+ S_0

E = -288.0344257 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.211061	-1.224596	0.000000
2	6	0	1.222147	0.168250	0.000000
3	6	0	0.000000	0.826284	0.000000
4	6	0	-1.219586	0.167154	0.000000
5	6	0	-1.209849	-1.227344	0.000000
6	6	0	0.000137	-1.917675	0.000000
7	1	0	2.149727	-1.764342	0.000000
8	1	0	2.161734	0.710666	0.000000
9	1	0	-2.160056	0.708723	0.000000
10	1	0	-2.148743	-1.766578	0.000000
11	1	0	0.001078	-3.000678	0.000000
12	7	0	-0.000924	2.323390	0.000000
13	1	0	0.469500	2.705387	0.828367
14	1	0	0.469500	2.705387	-0.828367
15	1	0	-0.959732	2.685267	0.000000

R = NH_3^+ T_1

E = -287.9050276 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.388097	1.031449	1.242143
2	6	0	0.388097	-0.332322	1.268441
3	6	0	0.099545	-1.021179	0.000000
4	6	0	0.388097	-0.332322	-1.268441
5	6	0	0.388097	1.031449	-1.242143
6	6	0	0.325338	1.736921	0.000000
7	1	0	0.515096	1.592131	2.161651
8	1	0	0.565023	-0.893930	2.179293
9	1	0	0.565023	-0.893930	-2.179293
10	1	0	0.515096	1.592131	-2.161651
11	1	0	0.360876	2.818910	0.000000
12	7	0	-1.338025	-1.645611	0.000000
13	1	0	-1.474832	-2.230313	0.830352
14	1	0	-2.068906	-0.919378	0.000000
15	1	0	-1.474832	-2.230313	-0.830352

R = NO_2 S_0

E = -436.8746215 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.210159	-1.821198
2	6	0	0.000000	1.218752	-0.429876
3	6	0	0.000000	0.000000	0.241543
4	6	0	0.000000	-1.218752	-0.429876
5	6	0	0.000000	-1.210159	-1.821198
6	6	0	0.000000	0.000000	-2.515492
7	1	0	0.000000	2.148743	-2.362381
8	1	0	0.000000	2.140336	0.135442
9	1	0	0.000000	-2.140336	0.135442
10	1	0	0.000000	-2.148743	-2.362381
11	1	0	0.000000	0.000000	-3.599387
12	7	0	0.000000	0.000000	1.722275
13	8	0	0.000000	-1.084435	2.290870
14	8	0	0.000000	1.084435	2.290870

R = NO_2 T_1

E = -436.7838219 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.037502	-1.839427	1.209523
2	6	0	0.037502	-0.451112	1.223736
3	6	0	0.032427	0.233112	0.000000
4	6	0	0.037502	-0.451112	-1.223736
5	6	0	0.037502	-1.839427	-1.209523
6	6	0	0.038220	-2.538018	0.000000
7	1	0	0.034887	-2.380374	2.148440
8	1	0	0.033442	0.104949	2.152441
9	1	0	0.033442	0.104949	-2.152441
10	1	0	0.034887	-2.380374	-2.148440
11	1	0	0.039765	-3.621400	0.000000
12	7	0	0.078798	1.627600	0.000000
13	8	0	-0.128247	2.380934	-1.042419
14	8	0	-0.128247	2.380934	1.042419

R = **NO** S_0

E = -361.6392457 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.767640	-1.679152	0.000000
2	6	0	-1.056864	-0.322920	0.000000
3	6	0	0.000000	0.596057	0.000000
4	6	0	1.329430	0.169254	0.000000
5	6	0	1.611567	-1.193856	0.000000
6	6	0	0.563938	-2.113925	0.000000
7	1	0	-1.571761	-2.406142	0.000000
8	1	0	-2.075494	0.045412	0.000000
9	1	0	2.115000	0.916226	0.000000
10	1	0	2.638875	-1.538512	0.000000
11	1	0	0.780880	-3.176303	0.000000
12	7	0	-0.183304	2.025387	0.000000
13	8	0	-1.335870	2.406108	0.000000

R = **NO** T_1

E = -361.6201979 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745151	-1.698463	0.000000
2	6	0	-1.051975	-0.345190	0.000000
3	6	0	0.000000	0.595178	0.000000
4	6	0	1.340888	0.166030	0.000000
5	6	0	1.620141	-1.191611	0.000000
6	6	0	0.583582	-2.130801	0.000000
7	1	0	-1.550787	-2.424318	0.000000
8	1	0	-2.077560	0.001850	0.000000
9	1	0	2.132959	0.904926	0.000000
10	1	0	2.652052	-1.523580	0.000000
11	1	0	0.810047	-3.190309	0.000000
12	7	0	-0.253169	1.952822	0.000000
13	8	0	-1.334930	2.523852	0.000000

R = CHO S_0

E = -345.6690898 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.615745	-1.229166	0.000000
2	6	0	-1.328147	0.133134	0.000000
3	6	0	0.000000	0.572544	0.000000
4	6	0	1.044087	-0.362714	0.000000
5	6	0	0.756104	-1.721117	0.000000
6	6	0	-0.573063	-2.154692	0.000000
7	1	0	-2.645021	-1.568996	0.000000
8	1	0	-2.132900	0.862091	0.000000
9	1	0	2.066296	-0.002758	0.000000
10	1	0	1.561635	-2.446690	0.000000
11	1	0	-0.794088	-3.216346	0.000000
12	6	0	0.286038	2.024994	0.000000
13	1	0	-0.617190	2.671949	0.000000
14	8	0	1.393202	2.515357	0.000000

R = CHO T_1

E = -345.5603218 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.635242	-1.206695	0.000000
2	6	0	-1.348913	0.146431	0.000000
3	6	0	0.000000	0.596510	0.000000
4	6	0	1.037105	-0.377167	0.000000
5	6	0	0.725126	-1.726867	0.000000
6	6	0	-0.605819	-2.157635	0.000000
7	1	0	-2.670055	-1.531163	0.000000
8	1	0	-2.153855	0.873391	0.000000
9	1	0	2.072062	-0.055765	0.000000
10	1	0	1.527830	-2.456292	0.000000
11	1	0	-0.838705	-3.215530	0.000000
12	6	0	0.281078	1.984408	0.000000
13	1	0	-0.507361	2.742382	0.000000
14	8	0	1.481259	2.511134	0.000000

R = $COCH_3$ S_0

E = -385.0016932 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.820999	1.276453	0.000008
2	6	0	-0.430565	1.191352	0.000001
3	6	0	0.204410	-0.057723	-0.000012
4	6	0	-0.579987	-1.219776	-0.000012
5	6	0	-1.966657	-1.134713	-0.000002
6	6	0	-2.590384	0.114520	0.000007
7	1	0	-2.302780	2.247606	0.000015
8	1	0	0.153979	2.103331	0.000001
9	1	0	-0.077372	-2.179248	-0.000022
10	1	0	-2.564298	-2.039311	-0.000004
11	1	0	-3.672703	0.181292	0.000015
12	6	0	1.698812	-0.204390	-0.000028
13	6	0	2.558587	1.046308	-0.000002
14	1	0	3.606030	0.749662	0.000044
15	1	0	2.355431	1.660481	-0.882101
16	1	0	2.355358	1.660500	0.882067
17	8	0	2.213383	-1.307063	0.000029

R = $COCH_3$ T_1

E = -384.8910246 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751777	-2.096441	0.000000
2	6	0	1.045506	-0.742404	0.000000
3	6	0	0.000000	0.222537	0.000000
4	6	0	-1.344573	-0.249857	0.000000
5	6	0	-1.613004	-1.607050	0.000000
6	6	0	-0.573688	-2.545727	0.000000
7	1	0	1.564821	-2.814463	0.000000
8	1	0	2.080281	-0.421591	0.000000
9	1	0	-2.159005	0.465590	0.000000
10	1	0	-2.643966	-1.944356	0.000000
11	1	0	-0.792631	-3.606699	0.000000
12	6	0	0.285195	1.610598	0.000000
13	6	0	1.664403	2.239254	0.000000
14	1	0	1.591049	3.327252	0.000000
15	1	0	2.219684	1.932275	0.892124
16	1	0	2.219684	1.932275	-0.892124
17	8	0	-0.671701	2.518032	0.000000

R = COOH S_0

E = -420.9481337 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.963454	-1.993959	0.000000
2	6	0	-1.125200	-0.611661	0.000000
3	6	0	0.000000	0.221681	0.000000
4	6	0	1.282741	-0.338202	0.000000
5	6	0	1.438883	-1.719657	0.000000
6	6	0	0.316241	-2.548520	0.000000
7	1	0	-1.834786	-2.638719	0.000000
8	1	0	-2.115112	-0.174660	0.000000
9	1	0	2.140702	0.322717	0.000000
10	1	0	2.433189	-2.151168	0.000000
11	1	0	0.438888	-3.625925	0.000000
12	6	0	-0.115802	1.703570	0.000000
13	8	0	0.816785	2.473291	0.000000
14	8	0	-1.403466	2.137131	0.000000
15	1	0	-1.369899	3.104862	0.000000

R = COOH T_1

E = -420.8228363 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.177087	-1.873182	0.000000
2	6	0	-1.234657	-0.525604	0.000000
3	6	0	0.000000	0.257704	0.000000
4	6	0	1.304697	-0.473213	0.000000
5	6	0	1.325451	-1.827580	0.000000
6	6	0	0.109521	-2.582547	0.000000
7	1	0	-2.089916	-2.458117	0.000000
8	1	0	-2.179358	0.000664	0.000000
9	1	0	2.206151	0.123760	0.000000
10	1	0	2.272906	-2.354714	0.000000
11	1	0	0.128006	-3.664097	0.000000
12	6	0	0.021332	1.690292	0.000000
13	8	0	1.049272	2.367993	0.000000
14	8	0	-1.219576	2.273093	0.000000
15	1	0	-1.070904	3.228607	0.000000

R = COOCH$_3$ S_0

E = -460.2581086 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.212201	1.236074	0.000000
2	6	0	1.391701	0.111590	0.000000
3	6	0	0.000000	0.262539	0.000000
4	6	0	-0.559670	1.545290	0.000000
5	6	0	0.263783	2.665951	0.000000
6	6	0	1.650554	2.512705	0.000000
7	1	0	3.289684	1.117030	0.000000
8	1	0	1.820711	-0.881602	0.000000
9	1	0	-1.638254	1.642857	0.000000
10	1	0	-0.173433	3.657840	0.000000
11	1	0	2.292477	3.386670	0.000000
12	6	0	-0.928278	-0.904103	0.000000
13	8	0	-2.135587	-0.820921	0.000000
14	8	0	-0.273805	-2.086552	0.000000
15	6	0	-1.102640	-3.262258	0.000000
16	1	0	-0.412493	-4.103176	0.000000
17	1	0	-1.734738	-3.283278	0.888808
18	1	0	-1.734738	-3.283278	-0.888808

R = COOCH$_3$ T_1

E = -460.1321388 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.089829	-1.423515	0.000000
2	6	0	0.753698	-1.245148	0.000000
3	6	0	0.193733	0.113250	0.000000
4	6	0	1.139714	1.267111	0.000000
5	6	0	2.474227	1.052124	0.000000
6	6	0	3.009068	-0.283289	0.000000
7	1	0	2.506274	-2.424568	0.000000
8	1	0	0.069145	-2.081882	0.000001
9	1	0	0.709892	2.259324	0.000001
10	1	0	3.159728	1.892205	0.000000
11	1	0	4.077875	-0.450179	-0.000001
12	6	0	-1.216964	0.386743	0.000000
13	8	0	-1.699852	1.517872	0.000000
14	8	0	-1.986616	-0.742904	0.000000
15	6	0	-3.403686	-0.524554	0.000000
16	1	0	-3.708457	0.032670	-0.887993
17	1	0	-3.851977	-1.516320	0.000000
18	1	0	-3.708457	0.032670	0.887993

R = $CONH_2$ S_0

E = -401.0702583 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.851513	1.226514	-0.139867
2	6	0	-0.458865	1.191823	-0.157200
3	6	0	0.219613	-0.024668	-0.016674
4	6	0	-0.516493	-1.205598	0.127328
5	6	0	-1.906615	-1.168596	0.154659
6	6	0	-2.577143	0.047675	0.022347
7	1	0	-2.368843	2.171376	-0.261727
8	1	0	0.090520	2.112949	-0.316263
9	1	0	0.021401	-2.141581	0.213754
10	1	0	-2.468457	-2.087882	0.275062
11	1	0	-3.660889	0.075834	0.038136
12	6	0	1.718702	-0.136704	-0.037506
13	8	0	2.285057	-1.181248	-0.314795
14	7	0	2.419032	1.007921	0.252917
15	1	0	1.986744	1.771662	0.745851
16	1	0	3.419726	0.909504	0.334604

R = $CONH_2$ T_1

E = -400.9435197 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.803203	1.279604	-0.063535
2	6	0	-0.475268	1.239643	-0.307774
3	6	0	0.253893	-0.038519	-0.155756
4	6	0	-0.552085	-1.284666	-0.121754
5	6	0	-1.879753	-1.211847	0.117421
6	6	0	-2.540564	0.067006	0.239825
7	1	0	-2.345174	2.216549	-0.135462
8	1	0	0.063758	2.128149	-0.614366
9	1	0	-0.028219	-2.223552	-0.238117
10	1	0	-2.470683	-2.117247	0.199892
11	1	0	-3.599369	0.117670	0.457032
12	6	0	1.685410	-0.129625	0.021234
13	8	0	2.274879	-1.217165	-0.083536
14	7	0	2.392975	1.049801	0.213057
15	1	0	1.935881	1.822862	0.673261
16	1	0	3.363373	0.914703	0.456676

R = CN S_0

E = -324.5777612 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.208739	-1.480787
2	6	0	0.000000	-1.215198	-0.090261
3	6	0	0.000000	0.000000	0.610288
4	6	0	0.000000	1.215198	-0.090261
5	6	0	0.000000	1.208739	-1.480787
6	6	0	0.000000	0.000000	-2.176538
7	1	0	0.000000	-2.147736	-2.021623
8	1	0	0.000000	-2.149097	0.457900
9	1	0	0.000000	2.149097	0.457900
10	1	0	0.000000	2.147736	-2.021623
11	1	0	0.000000	0.000000	-3.260446
12	6	0	0.000000	0.000000	2.042172
13	7	0	0.000000	0.000000	3.197850

R = CN T_1

E = -324.4545876 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	-1.251278	-1.460954
2	6	0	0.000000	-1.276992	-0.112992
3	6	0	0.000000	0.000000	0.651739
4	6	0	0.000000	1.276992	-0.112992
5	6	0	0.000000	1.251278	-1.460954
6	6	0	0.000000	0.000000	-2.190633
7	1	0	0.000000	-2.181198	-2.018217
8	1	0	0.000000	-2.206109	0.441961
9	1	0	0.000000	2.206109	0.441961
10	1	0	0.000000	2.181198	-2.018217
11	1	0	0.000000	0.000000	-3.272080
12	6	0	0.000000	0.000000	2.022817
13	7	0	0.000000	0.000000	3.201200